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EXPLAINABILITY INTERPRETABILITY AND SENSITIVITY ANALYSIS

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Advancing Machine Learning in Finance, Insurance and Economics

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SEMINAR OUTLINE

- Introduction
- Setup
- Sensitivity Analysis Settings (method-goal)
- Recent Advances
- Given Data Estimation
- Applications to Neural Networks

Brief Overview

Machine learning tools are increasingly applied in finance and insurance.

- Maldonado et al (2017)[1] use support vector machines for credit scoring;
- Fitzpatrick and Mues (2016)[2] review several classification algorithms for mortgage default predictions;
- Lessman et al (2017)[3] review classification algorithms for credit scoring;
- Atsalakis et al (2019)[4]: Neuro-fuzzy techniques for bitcoin price forecasting;
- Mai et al (2019)[5]: Deep learning for bankruptcy predictions;

- Nazemi et al (2018)[6]: Improving corporate bond recovery rate prediction using multi-factor support vector regressions
- Fisher and Krauss (2018)[7]: Deep learning with long short-term memory networks for financial market predictions
- Krauss et al (2017)[8]: Deep neural networks, gradient-boosted trees, random forests: Statistical arbitrage on the S&P 500

SCIENTIFIC SIMULATORS

A scientific model is built to help the interested user (a scientist, a decision maker) in gaining insights on a given problem. The problem can be the behavior of a physical or socio-economic system or the identification of the best policy among a set of given strategies.

Ideally, a model follows from an overarching theory, which determines the hypothesis under which the model is valid or "true", and characterizes mathematically the behavior of the phenomenon or system of interest.

In machine learning, the model is often fitted to the data in order to gain managerial or scientific insights.

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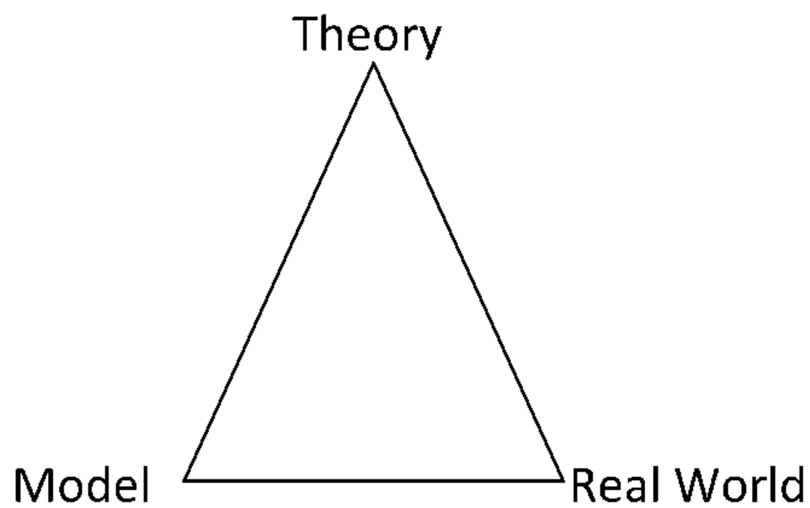
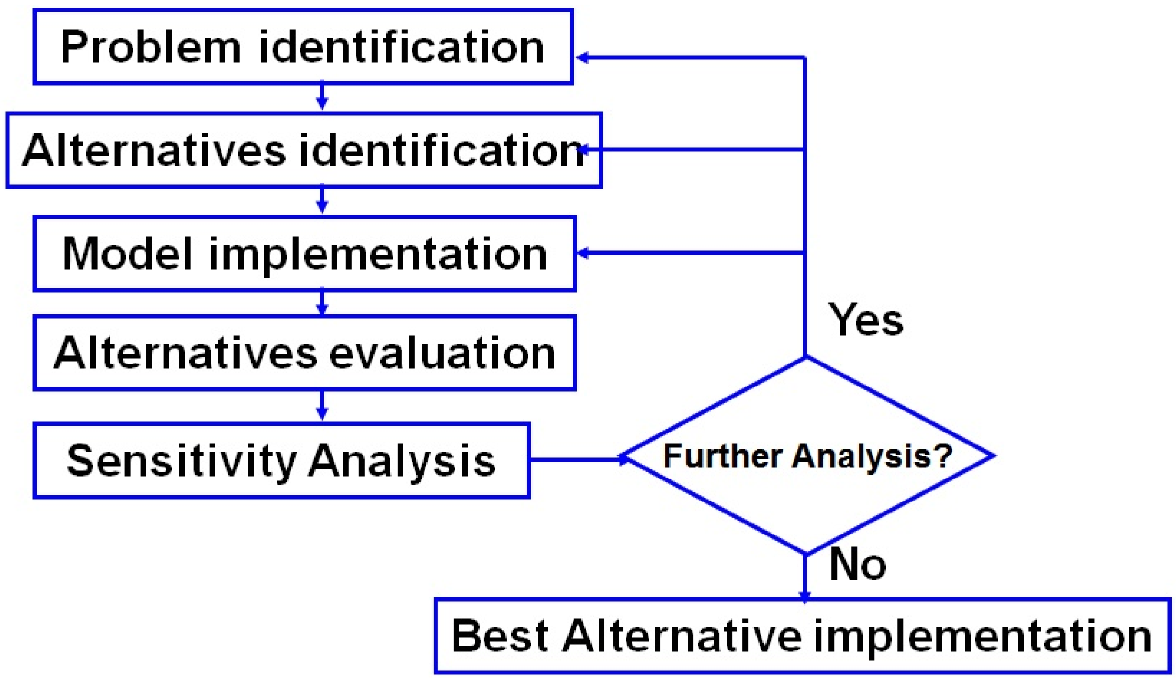
THE SCIENTIFIC FRAMEWORK



The "Vienna School" scientific triangle (see also B. 2017)[9].

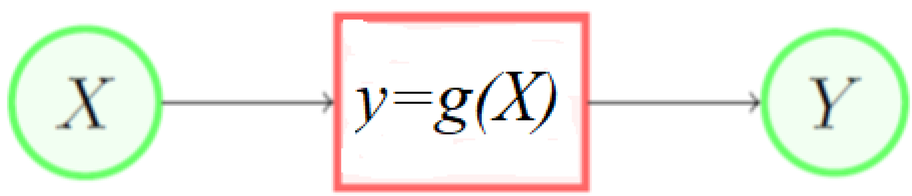
THE DECISION-MAKING PROCESS



From Figure 1.1 in Clemen (1997)[10].

SETUP

Simulators or Machine Learning tools try to quantify the relationship under “nature” creating an input output mapping:



(see [11] among others; the first graph is taken from such source).

SETUP (CONT.)

The input-output mapping estimates one or more quantities of interest (y) given a vector of inputs ($\mathbf{x}$):

$$y = g(\mathbf{x})$$

In several situations there is uncertainty about the inputs and this may even combine with a stochastic response.

The model output becomes a random variable with a distribution $F_y(y)$ (density $f_y(y)$).

THE BLACK BOX MENACE

(Begoli, Bhattacharya, and Kusnezov 2019, p. 21) underline the issue that the "Absence of Theory" makes a proper uncertainty quantification an essential ingredient in the use of black-box machine learning algorithms.

[13] suggests that interpretability and explainability issues impact the use of artificial intelligent methods.

[14] underlines that modelling quality and validity is at stake, especially as model complexity increases

… AND MORE

- Scientific models are expensive (modelling teams devote much time and resources) to build
- The input-output mapping is often not known analytically
- The limits of the model response and its prediction accuracy are often unknown.

A process needs to start to find out what it was about the inputs that made the output came out as they did (Little 1970) [15]

… and more

Rudin (2019)[16]

- Black box models because of proprietary reasons and not because of intrinsic complexity
- Examples in credit scoring
- Proprietors not willing to open the model
- High-stake decisions

A process needs to start to find out what it was about the inputs that made the output came out as they did (Little 1970) [15]

SENSITIVITY ANALYSIS AND MODEL INFERENCE

Guidotti et al(2018)[13], Saltelli (2019)[14] suggest sensitivity analysis as an essential part of scientific modelling to:

- Increase transparency
- Enhance interpretability and explainability
- Increase awareness of the model behavior

FOR THE ANALYST

There are several methods that, if properly used, help the analyst in:

- increasing awareness about the model behavior
- understanding the model limitations
- understanding areas where further modelling efforts are needed
- redirecting new information collection towards important features
- properly communicating results to the decision maker

FOR THE DECISION MAKER

A proper sensitivity analysis:

- Helps the decision-maker in asking the right questions to the model (with the help of the analyst)

- Allows to rigorously identify the factors on which to focus managerial attention before and after the decision

CURRENT PRACTICE?

The recent investigation of Saltelli et al (2019)[17] suggest that most scientific works using mathematical modelling either do not perform a sensitivity analysis or, if they perform one, the use very simple one-at-a-time methods.

For instance, the very recent work of de Graf et al (2019)[18]: "A one-at-a-time sensitivity analysis showed that varying model parameters (hydraulic conductivity and surface-water depths) or using different climate models changed the number of watersheds and timing of environmental limits reached (see Methods)."

DRAWBACKS

-OAT is the first thing that comes into mind

- There is no “method-Goal” approach

- Sensitivity analysis is then not entirely helpful

SENSITIVITY ANALYSIS QUOTES

The judicious application of sensitivity analysis techniques appears to be the key ingredient needed to draw out the maximum capabilities of mathematical modeling (Rabitz 1989[19], p. 221).

Sensitivity Analysis for Modelers: Would you go to an orthopedist who did not use X-Ray? (Fuerbinger 1994)[20].

In order for the analysis to be useful it must provide information concerning the way in which our equilibrium quantities will change as a result of changes in the parameters (Samuelson 1941, p. 97)[21].

GOALS

FACTOR PRIORITIZATION

The factor prioritization setting is associated with obtaining insights about the most important model inputs.

Under uncertainty, these insights need to be obtained using a global sensitivity method.
Under certainty, and if one is considering finite changes in the model inputs, finite scale sensitivity indices are appropriate tools.
Infinitesimal perturbations are of concern, then differentiation-based sensitivity measures are appropriate.

MODEL STRUCTURE

In a model structure setting, analysts are interested in determining whether the model response is the sum of the individual model inputs or whether interactions play a relevant role.

The sensitivity measures appropriate for this setting depend on the scale of the investigation (e.g., Hessians on a local scale, finite change sensitivity indices or high order variance-based sensitivity indices)

TREND DETERMINATION

In a model structure setting, analysts are interested in determining whether the model response is the sum of the individual model inputs or whether interactions play a relevant role.

The sensitivity measures appropriate for this setting depend on the scale of the investigation (e.g., Hessians on a local scale, finite change sensitivity indices or high order variance-based sensitivity indices)

STABILITY

In a stability setting we are interested in understanding whether the optimal solution or an equilibrium is stable (or not) given variations in the exogenous vactors.

METHODS

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DIFFERENTIAL SENSITIVITY ANALYSIS

Cox and Baybutt (1981)[22], Frey and Patil (2002,2004)[23,24], B. (2008)[25], Riedmann et al (2015)[26] in occupational exposure modeling, Percoco 2011[27] in input-output modeling; Tsanakas and Millossovich (2016) [28] Antoniano et al. (2018)[29] on stochastic simulators.

From B. 2008:

$$D_i = \frac{g_i^{'} dx_i}{\sum_{j=1}^{n} g_j^{'} dx_j}$$

$$D_i = g_i^{'} \text{ if uniform parameter changes}$$

$$D_i = E_i^{'} \text{ if proportional parameter changes}$$

Derivative-based methods require differentiation algorithms

INSIGHTS FROM DIFFERENTIAL METHS.

1) Trend Determination: Signs of partial derivatives provides indication about trend
2) Factor Prioritization: Magnitude of Differential Importance provides indication about the relevance of the inputs.
3) Interaction quantification if second order partial derivatives are computed as well

Notes:

a) Partial derivatives not comparable, thus not for factor prioritization, unless the inputs are denominated in the same units; one uses elasticities instead

b) Can be randomized to give rise to derivative-based global sensitivity measures (a bridge between local and global methods)

REGRESSION-BASED SA METHODS

Among the first methods used (works of Helton, Kleijnen and several others[30–33]). Intuition:

$$y \simeq \beta_0 + x_1\beta_1 + x_2\beta_2 + \ldots + x_n\beta_n + \epsilon$$

The response surface can be well approximated by a linear regression.

Then, natural sensitivity measures become the standardized regression coefficients (SRC):

$$SRC_i = \frac{\beta_i \cdot \sigma_i}{\sigma_Y}$$

Note that if the linearity assumption holds, we have

$$\sum_{i=1\ldots n} SRC_i^2 = \sigma_Y^2$$

where σ_Y^2 is the variance of the model response.

VARIANCE-BASED SENSITIVITY MEASURES

To overcome SRC limitations for nonlinear models, Iman and Homma (1990) define variance-based sensitivity measures

$$V_i = \mathbb{V}[\mathbb{E}[Y \mid X_i]]$$

The same intuition of sensitivity measures can also be found outside the Risk Analysis field, in Sobol' (1990)[34], Wagner (1995)[35], Homma and Saltelli (1996)[36], Pearson (1905)[37].

Iman and Hora also address estimation accuracy and the use of monotonic transformations of the output.

Variance-based sensitivity measures have, since then, be used in several quantitative risk assessment studies.

NULLITY IMPLIES INDEPENDENCE

Renyi's 1959[38] postulate D: a measure of statistical dependence should possess the property that it is zero if an only if *Y* is independent of X_i.

It turns out that first order variance-based sensitivity measures, as well as standardized regression coefficients do not possess this property.

MOMENT-INDEPENDENT SENSITIVITY MEASURES

Moment independent sensitivity measures are importance measures that consider the entire distribution of the model output.

- An early moment independent sensitivity measure is the δ-importance measure (B. 2006, B. et al 2011, Wei 2014[39–41])

$$\delta_i = \frac{1}{2}\mathbb{E}_i\left[\int_{\mathcal{Y}} | f_Y(y) - f_{Y|X_i}(y;x_i) | dy\right]$$

This importance measure is based on the L1-norm between densities. δ_i is monotonic transformation invariant

1) $\delta_{1,2,\ldots,n} = 1$: the importance of all inputs is unity

2) $\delta_i = 0$ if and only if Y is independent of X_i .

3) δ_i is transformation invariant

TRANSFORMATION INVARIANCE

Iman and Hora (1990): “The scaling problem most often can be overcome by performing uncertainty importance calculations based on a logarithmic scale for the top-event frequencies … However, the log-based uncertainty importance calculations do not readily translate back to a linear scale.”

The issues are overcome if the sensitivity method is transformation invariant (B. et al. 2014[42]).

OTHER M-I SENSITIVITY MEASURES

$\delta_i^{KL} = \mathbb{E}[\int_{\mathcal{Y}} f_Y(y) \ln \frac{f_Y(y)}{f_{Y|X_i}(y)} dy]$ based on the Kullback-Leibler divergence

$\beta_i^{KS} = \mathbb{E}_i[\sup_{\mathcal{Y}} | F_Y - F_{Y|X_i} |]$ based on the Kolmogorov-Smirnov distance

$\beta_i^{Ku} = \mathbb{E}_i[\sup_{\mathcal{Y}}\{F_Y - F_{Y|X_i}\} + \sup_{\mathcal{Y}}\{F_{Y|X_i} - F_Y\}]$ based on the Kuiper distance

$\beta_i^{CvM} = \mathbb{E}_i[\int_{\mathcal{Y}} \left(F_Y(y) - F_{Y|X_i}(y)\right)^2 dy]$ based on the Cramer-Von Mises distance

THE COMMON RATIONALE

Variance-based, as well as all moment independent sensitivity measures above can be written in the following form:

$$\xi_i = \mathbb{E}_i[d(\mathbb{P}_Y, \mathbb{P}_{Y|X_i})]$$

with $d(\cdot,\cdot)$ generic operator between any property of the marginal ($\mathbb{P}_Y$) or conditional distribution of Y ($\mathbb{P}_{Y|X_i}$).

This Common Rationale (B. et al 2016)[43] allows one to find the following result:

A global sensitivity measure in the common rationale possesses the nullity-implies independence property if and only if it considers the entire distribution of the model output.

VALUE OF INFORMATION

$$\epsilon_i = \min_{a \in A} \mathbb{E}[\mathcal{L}(Y)] - \mathbb{E}_i\{\min_{a \in A} \mathbb{E}[\mathcal{L}(Y) \mid X_i]\}$$

Difference between the loss given that we do not know and the loss given that we know X_i.

Among the several properties: $\epsilon_i \geq 0$. However, ϵ_i does not share the nullity implies independent property.

GIVEN DATA ESTIMATION

Thanks to the common rationale, we can write:

$$\hat{\xi}_i = \frac{\sum_{m=1}^{M} \overset{\frown}{p}_m^{\,i} d(F_Y, F_{Y|X_i \in \mathcal{C}_m})}{M}$$

- [43] show that under mild conditions the above estimator converges to the true value as the sample size increases.
- Computational Cost: *N* model runs, independent of the dimensionality of the model

AN APPLICATION:

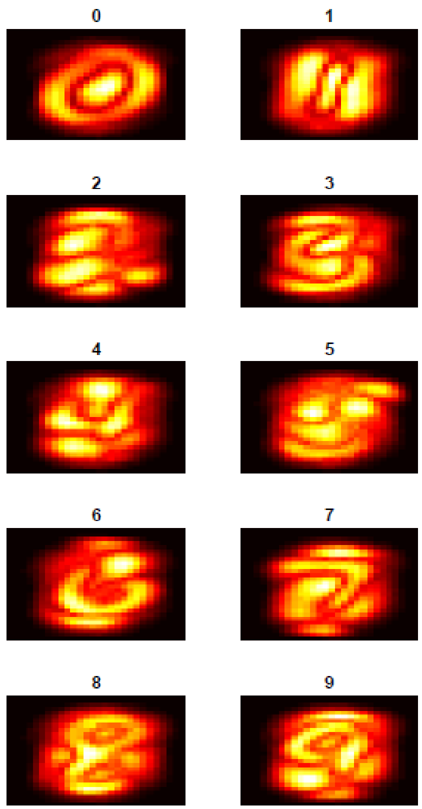
Do Deep Neural Networks See Statistical Dependence?

MNIST DATASET

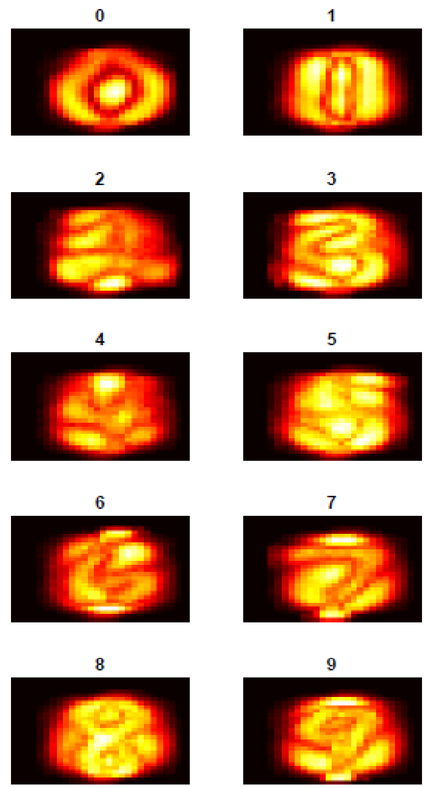
Pixels $\rightarrow$ Inputs (X)

Output: Classification Score

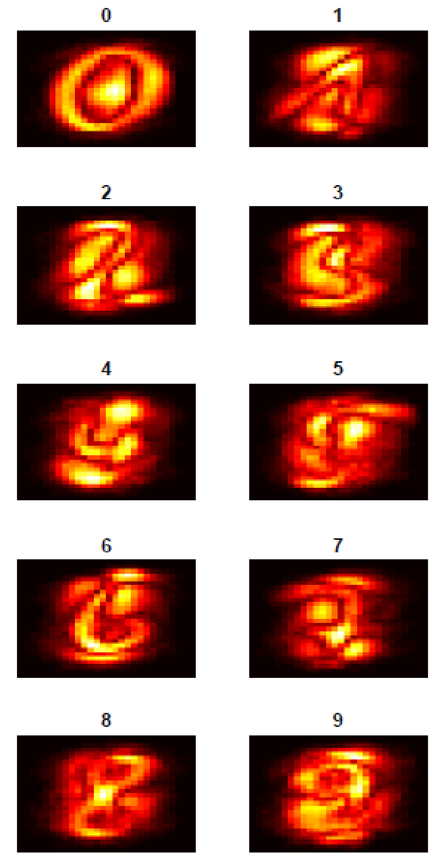
STATISTICAL HEATMAPS



(a) MNIST Database



(b) USZIP Database



(c) Seewald Database

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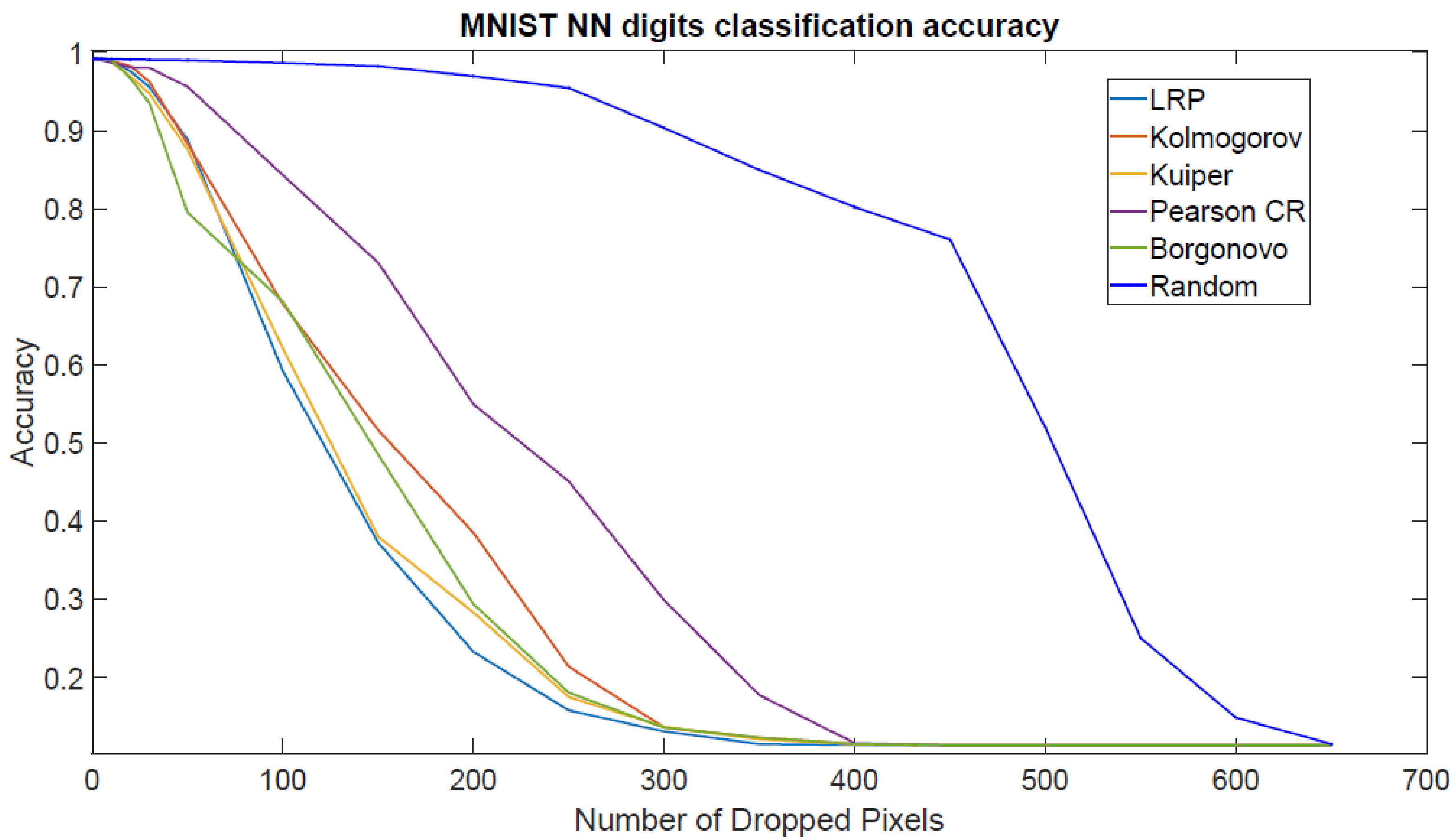
DROPPING PIXELS MNIST



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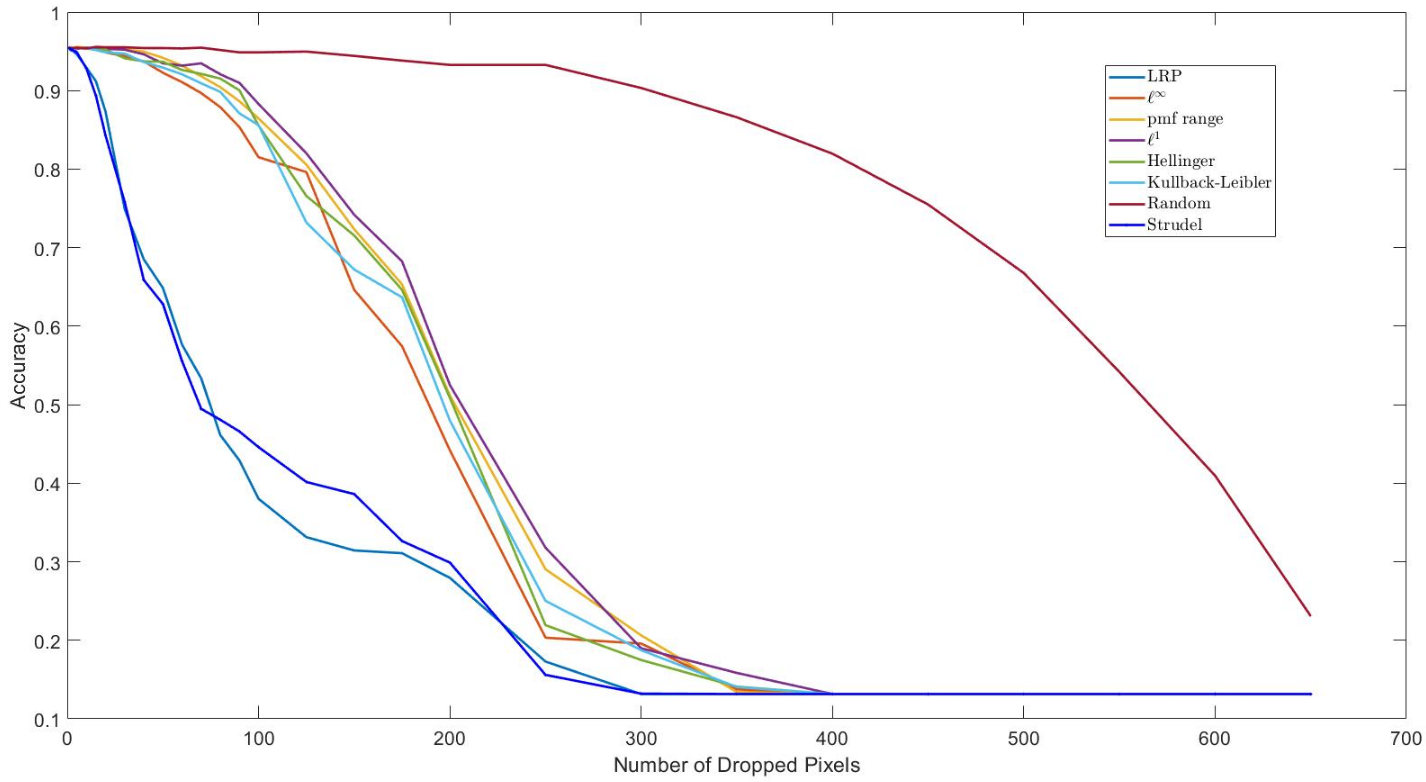
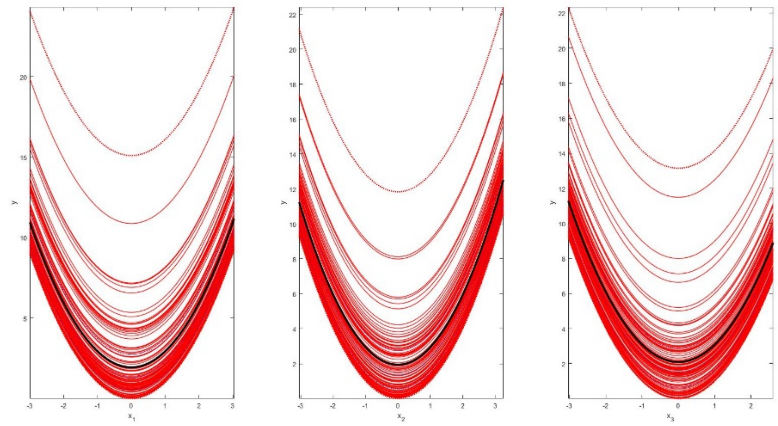
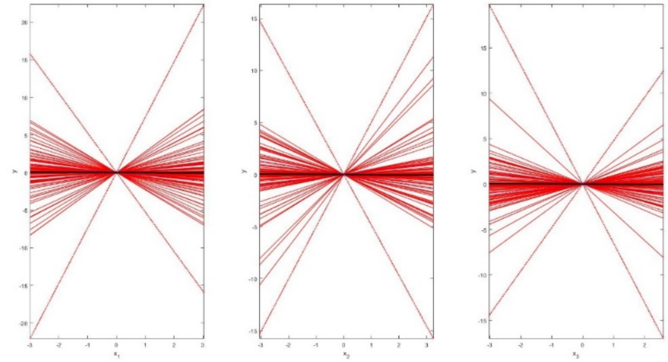
DROPPING PIXELS USZIP



DOES YOUR OUTPUT BEHAVE LIKE THIS?



OR LIKE THIS?



UNDERSTANDING TREND

Understanding whether the model responds positively or negatively to input variations.

It is essential for:

1) Model debugging (is the response coherent with intuition? Is there an error in the code?)
2) Managerial action: if a variable has a positive impact, action must be taken to guarantee the variable does not decrease
3) Policy implementation

FOCUS ON
GLOBAL TREND INDICATORS

Conditional Regression Curves[44]

$$r_i(x_i) = \mathbb{E}[g(\mathbf{X})|X_i = x_i] = \int_{\mathcal{X}_{\sim z}} g((\mathbf{x}_{-i}; x_i))dF_{\mathbf{X}|X_i}(\mathbf{x}_{-i}; x_i)$$

Partial dependence functions[45]

$$h_i(x_i) = \int_{\mathcal{X}_{\sim i}} g(x_i; \mathbf{x}_{\sim i})dF_{\mathbf{X}_{\sim i}}(\mathbf{x}_{\sim i})$$

THE FUNCTIONAL ANOVA EXPANSION

Functional ANOVA: $$g(\mathbf{x}) = \sum_{z \subseteq \{1,2,\ldots,n\}} g_z(\mathbf{x}_z)$$

First order terms under independence[46,47]:

$$g_i(x_i) = \mathbb{E}[g(\mathbf{X})|X_i = x_i] - g_0 = r_i(x_i) - g_0$$

First order term under dependence as in Hooker (2007)[48,49]

$$g_i\ (x_i) = \int_{\mathcal{X}_{\sim i}} g(\mathbf{x}) dF_{\sim i}(\mathbf{x}_{\sim i}) - g_0 - \sum_{\{i\} \subset v \in 2^Z} \int_{\mathcal{X}_{\sim i}} g_v(\mathbf{x}_v) dF_{\sim i}(\mathbf{x}_{\sim i}).$$

The first addendum is a partial dependence function:

$$g_i(x_i) = \int_{\mathcal{X}_{\sim i}} g(x_i;\mathbf{x}_{\sim i}) dF_{\mathbf{X}_{\sim i}}(\mathbf{x}_{\sim i}) = h_i(x_i) - g_0 - q_i(x_i)$$

CONSISTENT INDICATORS

Definition: *We say that an indicator of trend is consistent if the following happens: Given that* g *is monotonic (convex), then also the conditional regression lines are monotonic and convex.*

Proposition:

a) *Independent inputs:* $r_i(x_i)$ *and* $h_i(x_i)$ *are consistent with respect to the trend and convexity of g.*

b) *Dependent inputs but Cartesian Domain:* $h_i(x_i)$ *remain consistent*

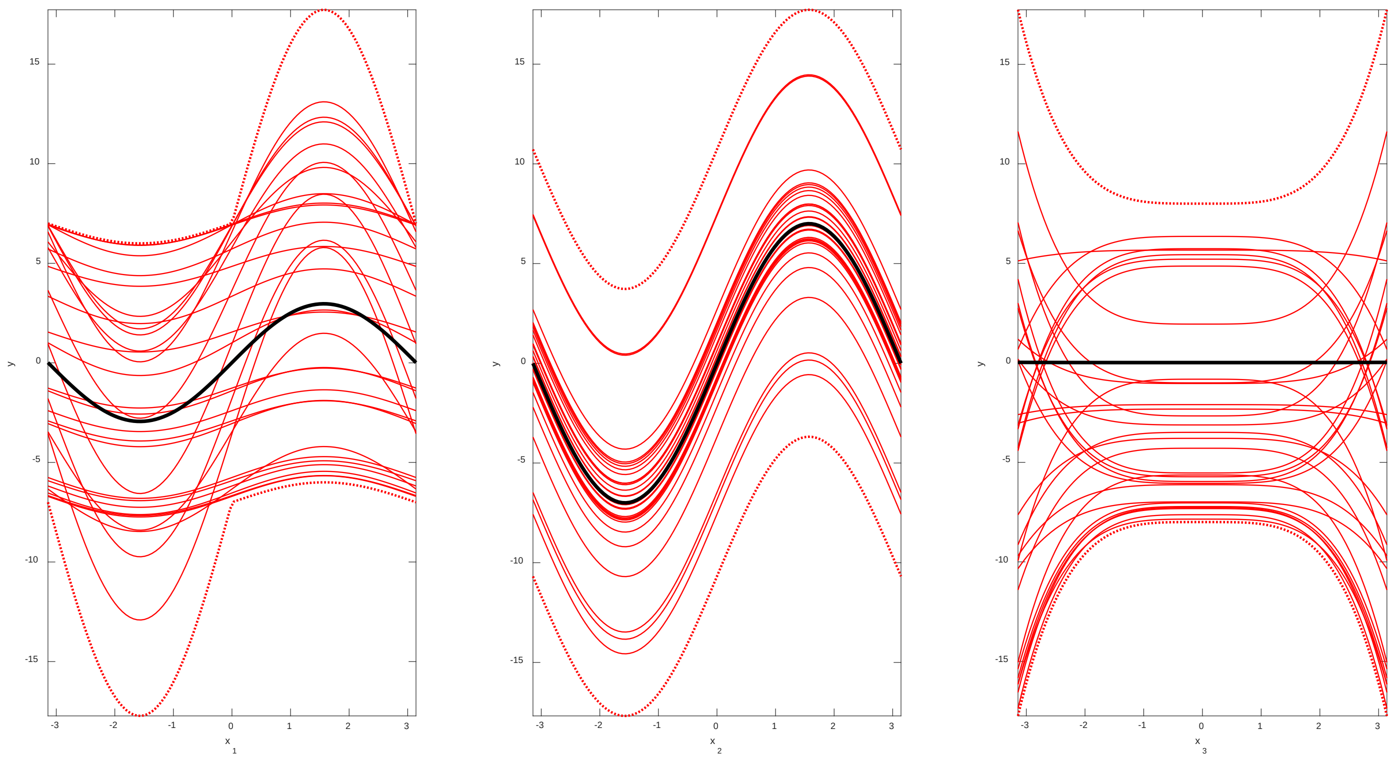
c) *Constrained inputs: neither* $h_i(x_i)$ *nor* $r_i(x_i)$ *are consistent*

Proof in B. et al (2019)[50].

EXAMPLE

Consider the input-output mapping

$$y = sin(x_1)(1+0.1x_3^4) + 7sin(x_2)^2$$



SUMMARY FOR A SET OF TREND INDICATORS

Measure	Symbol	Data	Cost	Safeguard	Discrete	Handles Uncertainty
Pearson's corr. coeff.	ρ_{YX_i}	Yes	N	Independence	Yes	Yes
Spearman's rank corr. coeff.	$\rho_{YX_i}^{Sp}$	Yes	N	Independence	Yes	Yes
Conditional regression curve	r_i	Yes	N	Independence	Yes	Yes
Partial dependence function	h_i	Yes	nKN, N	Always	Yes	Yes
Partial derivative	g_i'	No	$N(n+1)r$	Always	No	If randomized
Mixed derivative	$g_{i,j}'$	No	r	Always	Yes	If randomized
One-way function	w_i^0	No	r	Always	Yes	If randomized

UNDERSTANDING STRUCTURE

Question: if two or more variables vary simultaneously, does their joint variation produce a synergistic (positive interaction) or an antagonistic effect?

Answering the question is important both for the analyst (does the model comply with intuition or with an underlying theory?) and for the decision-maker (protecting/exploiting joint variations)

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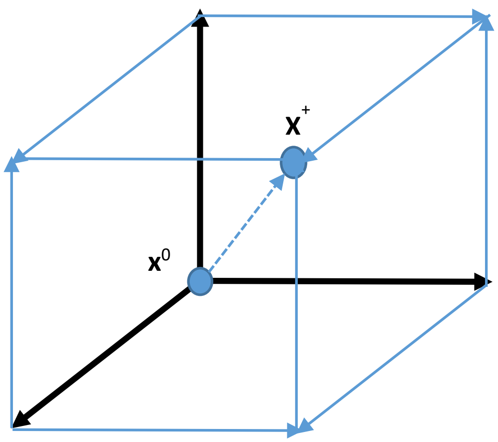
TOOLS FOR UNDERSTANDING INTERACTIONS

Infinitesimal scale: Second order Partial derivaties

Finite scale: Finite Change Sensitivity Indices (B. 2010, Risk Analysis)[51]

Global Scale: Sobol' indices (Sobol 1993), Effective Dimensions (Owen 2003), Total Indices (Homma and Saltelli 19969, Shapley Values (Rabitti and B. 2019)

FINITE CHANGE DECOMPOSITION



$$\Delta y = g(\mathbf{x}^{+}) - g(\mathbf{x}^{0})$$

How do we explain this change?:

FINITE CHANGE DECOMPOSITION (Cont.)

$$\Delta y = \sum_{i=1}^{n} \phi_i + \sum_{i<j} \phi_{i,j} + \ldots + \phi_{1,2,\ldots,n}$$

where

$$\begin{cases} \phi_i = g(x_i^+; \mathbf{x}_{\sim i}^0) - g(\mathbf{x}^0) \\ \phi_{i,j} = g(x_i^+, x_j^+; \mathbf{x}_{\sim i,j}^0) - \phi_i - \phi_j - g(\mathbf{x}^0) \\ \phi_{i,j,k} = g(x_i^+, x_j^+, x_k^+; \mathbf{x}_{\sim i,j,k}^0) - \phi_{i,j} - \phi_{i,k} - \phi_{j,k} - \phi_i - \phi_j - \phi_k - g(\mathbf{x}^0) \\ \ldots \end{cases}$$

$\phi_{i,j}$ is a second order interaction index between X_i and X_j.

INFINITESIMAL SCALE

$$Y''_{i,j} = \lim_{h_i, h_j \to 0} \frac{\phi_{i,j}}{h_i h_j}$$

where

$$g(x_i^{\,0} + h_i, x_j^{\,0} + h_j; \mathbf{x}^0_{-i,j}) - g(x_i^{\,0} + h_i; \mathbf{x}^0_{-i}) - g(x_j^{\,0} + h_j; \mathbf{x}^0_{\;j}) + g(\mathbf{x}^0)$$

Thus, on the infinitesimal scale, interactions are associated with convexity/concavity.

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GLOBAL SCALE II

Efron and Stein (1981)[46] prove that a multivariate mapping g, square integrable on $(\mathcal{X}, \mathcal{B}(\mathcal{X}), \mu)$, can be decomposed as follows:

$$g(\mathbf{x}) = g_0 + \sum_{i=1}^{n} g_i(x_i) + \sum_{i<j} g_{i,j}(x_i, x_j) + \ldots + g_{1,2,\ldots,n}(x_1, x_2, \ldots, x_n)$$

where

$$\begin{cases} g_0 = \iint g(\mathbf{x}) d\mu \\ g_i(x_i) = \iint g(\mathbf{x}) \prod_{k \neq i} d\mu_k - g_0 \\ g_{i,j}(x_i, x_j) = \iint g(\mathbf{x}) \prod_{k \neq i,j} d\mu_k - g_i(x_i) - g_j(x_j) - g_0 \\ \ldots \end{cases}$$

GLOBAL SCALE III

Variance decomposition

$$\mathbb{V}[Y] = \sum_{s=1}^{n} V_s + \sum_{s<j} V_{s,j} + \sum_{s<j<m} V_{s,j,m} + \ldots + V_{1,2,\ldots n}$$

$$V_{s,j\ldots,m} = \int \ldots \int \left[g_{s,j\ldots,m}(x_s, x_j, \ldots, x_m) \right]^2 \prod_{k=s,j,\ldots,m} dF_{X_k}$$

SOURCES OF INTERACTIONS

Interaction terms: $\mathbb{E}[Y \mid X] = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{1,2} X_1 X_2$

Context-Specific Interactions: jumps

Spurious Interactions: Correlations

AN OVERVIEW

Challenges: Computational Burden

Finding the Appropriate Tool

Scale	Inter.Term	Piec.-def.	Spurious	Sign	Discreteness	Cost	Assumption on g
Infinitesimal	Yes	No	No	Yes	No	$4nN$	Differentiability
Finite Change	Yes	Yes	No	Yes	Yes	2^n	Existence
Global	Yes	Yes	Yes	No	Yes	$N^2 2^n$	Square Integrability

OTHER BROAD CHALLENGES

Running times and Dimensionality: Given data approaches.

- Emulation
- Partition-based Estimation

Faster Kriging method recently introduced (Lu et al. 2019)[52] allows kriging up to 40000 variables.

Uncertainty in the estimates (Bayesian non-parametric approaches to obtain confidence intervals in the estimates (Le Gratiet et al. (2014)[53], Antoniano et al. 2019)[54]).

CONCLUSIONS

Rich interchange between Mathematical Modelling and Sensitivity Analysis.

The availability of Sensitivity Analysis methods helps the analyst and the decision-maker in better understanding results.

Perhaps not a key to interpretability or explainability, but definitely a set of tools that help the modeler.

THANK YOU
FOR
YOUR ATTENTION!

Slides and codes are available

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